4.3 Provisional Guidance for the Initial Assessment of Environmental Exposure*

4.3.1 Introduction

1. This document provides guidance for the application of simple models for the initial assessment of environmental exposure of High Production Volume (HPV) chemicals for which a full SIDS is available, based mainly on the conclusions and recommendations of the OECD Workshop on the Application of Simple Models for Environmental Exposure Assessment (Berlin, 11-13 December 1991).

2. The objective of the Workshop was to identify simple models which can be used for initial environmental exposure assessment of new and existing chemicals with limited data including indirect exposure to man via food and drinking water, in particular those models which can be used in the context of the OECD work on HPV chemicals. This means that the models should be applicable using data which are available in the SIDS. One further objective was to develop guidance for Member countries in using these models when they develop their recommendation related to the initial assessment of SIDS chemicals.

3. An exposure assessment consists of a source assessment and a fate and pathway assessment (Ref. 38 and 16). In a source assessment, identification of emission source(s) and an estimation of release(s) from the source(s) are made by means of information on use categories of a chemical and emission factors generally. Exposure through the environment (environmental exposure) is considered in a fate and pathway assessment. Then indirect exposure through food and drinking water is calculated based on these results. This document focuses on three issues in this procedure: emission factors and use categories, simple models for environmental exposure, and models for indirect exposure.

4. It should be noticed that the overall environmental exposure assessment should strive to conduct an assessment at the global level. Even though the exposure situation to a chemical might be different depending on local or national conditions, all calculations at these levels should be integrated in the global assessment.

5. Also it is important to consider a variety of emission sources and to include several sources in the assessment. To date, environmental exposure assessments dealt with by the SIDS Initial Assessment Meeting (SIAM) almost always considered emission data from a single point source, e.g. one production site, though various sources such as other producers, subsequent processing independent of the producer, and produced product are considered to exist. When several sources cannot be considered qualitatively in the assessment, a more simple qualitative approach such as a scoring system might be considered.

6. Following the recommendations of the Berlin Workshop, diskettes with national models that were thought to be appropriate for initial assessment of HPV chemicals with full SIDS at the Workshop have been prepared and distributed separately with an explanatory note which includes manuals of each model (Ref. 35, details in Ref. F). Also local and global reference models, which could be used in addition to and/or in place of national models, have been developed based on the recommendations of the Workshop and have been distributed by means of a diskette (Ref. 36 and 37, details in Ref. F).

7. In addition, Discussion Documents (Ref. 14, 16, 18, 19) and Background Documents (Ref. 20-22) prepared for the Workshop could be referred to whenever detailed information relating to the assessment procedure presented in this document is required. These documents were prepared on the basis of information on the procedures and the results of the application of ten Member countries' approaches on ten SIDS chemicals (Ref. 1-13) and are included in Environment Monograph No. 67 (Ref. 38).

8. Structure-Activity Relationships (SARs) for physical-chemical properties important for exposure assessment were also addressed at the Workshop (Ref. 17) and the report has been distributed separately as an Environment Monograph (Ref. 39).

4.3.2 Emission Factors and Use Categories of Chemicals

* This document was prepared by the OECD Secretariat in 1992 based on the OECD Workshop on the Application of Simple Models for Environmental Exposure Assessment, held in Berlin in December 1991. It has been updated to reflect comments by Member countries and agreements reached in the context of the OECD Existing Chemicals Programme up to mid-1994.

9. Release of chemicals into the various environmental compartments and the quantities concerned are strongly dependent on the use of the chemical. Therefore, in an exposure assessment, the use pattern of a substance should be considered as a starting point when using any kind of exposure scenario. When high quality information and data are lacking, screening quality release assessments can be made by using a typical or average release scenario based on emission factors presenting a boundary estimate of release of chemicals. It should be noticed that the results of the source assessment are used as input data for models for environmental and indirect exposure assessment.

10. "Emission Factors and Use Categories" (Ref. 14 and 38) present various approaches used in Member countries, and detailed information is provided in Ref 20. The tools mentioned in the documents will assist Member countries in developing release assessments, as well as allow them to understand the assessments of other Member countries. The summary report of the Working Group on this issue of the Workshop is attached to this document as Annex 1.

Necessary Information for Source Assessments

11. Initial exposure assessments can often be based on the SIDS Dossier. However, in order to improve the quality of the assessment, further information on exposure and use are considered to be necessary and elements of exposure information have been agreed and are included in the SIDS (see Section 2.2).

12. In order to collect the necessary information, release reporting requirements such as a product register system would be a good source of information. In addition, manufacturers could provide more detailed information on chemical use and releases, and monitoring data could be collected intensively. Data from monitoring should be used as much as possible, in order to compare them with the results obtained from other methods such as emission scenario approaches.

Assessment Methods for Release of Chemicals

13. Approaches of Member countries for estimating releases of SIDS chemicals into water, which were discussed at the Workshop, are often conceptually similar. However, differences in values chosen for variables contained in release calculations frequently lead to widely varying release concentrations. This situation probably exists for other release scenarios that may be evaluated in the future. There is a clear need for Member countries to work more closely together to develop mutually compatible release estimation methods.

14. Releases should be assessed for the entire life-cycle of SIDS chemicals. The life-cycle of a chemical includes:

-- manufacture or production;
-- processing or formulation;
-- industrial use;
-- private or consumer use;
-- recycling; and
-- disposal and treatment.

15. For commonly encountered release scenarios, estimates of releases can be presented in the form of the matrix shown in the Appendix to Annex 1 to this document, which shows releases as a fraction of production or use volume.

16. All SIDS release assessments should be extremely clear with regard to how they were developed and should, when possible, include:

-- rationales, assumptions and data used to generate release estimates;
-- types of releases (point source or diffuse);
-- release quantities;
-- media for release;
-- time dimensions of releases;
-- kinds of release estimates (average or worst case); and
-- uncertainties associated with the estimates.

17. Release assessments address releases up through waste water treatment. Water releases of SIDS chemicals are estimated before and after waste water treatment.

18. The SIDS assessment efforts should be structured to avoid false negatives - incorrectly excluding chemicals of potential concern from further consideration, for example, by considering a worst case scenario.

19. An iterative approach to improving initial assessments may be needed on occasion.

4.3.3 Local Models and Global Models

20. The environmental exposure assessments are generally carried out by means of models and are based on information obtained by a source assessment, as well as on information on the properties of the chemical and on the environment for which estimations will be made. Application of local and global models for a chemical is considered depending upon production and use of the chemical, in order to discriminate local exposure and general exposure. In this document local models are those which are concerned with the environment close to the release site, and with a short time scale after the release. They can use environmental data which are generic, or they can use data from a real situation if such data are available. On the other hand, global models are those which are concerned with the longer term, steady-state behaviour of a chemical and are multi-media. The estimated concentrations of a chemical in the environmental media are used for comparison with "a low risk level of a chemical" derived from an effects assessment. An elaborated exposure assessment based on more precise and detailed information and/or a refined effects assessment would be required in cases where estimated concentrations exceed the "low risk level of the chemical".

21. Diskettes which compile national and reference models could be used for the actual estimation of the concentration of a chemical (see Ref. F).

22. "Local and Global Models" (Ref. 16 and 38) introduces a procedure for SIDS initial assessment and the issues to be considered in an environmental exposure assessment. Reference models which would be used for the initial environmental exposure assessment are presented in the document, "Reference models which would be used for the Initial Environmental Exposure Assessment" (Ref. 19 and 38). Outlines of national models and results of their application for ten SIDS chemicals are summarized in "Local and Global Models in Member countries" (Ref. 21 and 38). "Potential Approaches for Developing Screening-Level Environmental and Human Exposure Assessment for SIDS Chemicals" (Ref. 22 and 38), which can be applied when sufficient information on the source and the environment are available, presents an approach taken by the US. The summary report of the Working Group is attached to this document as Annex 2.

Necessary Information for Models

23. The physical-chemical data available in the SIDS are generally sufficient for using local and global models used for the initial assessment. Information on degradation rates is generally missing in the SIDS although they are included implicitly. This might be a problem for global models. Also the release estimates in the previous section should be able to be used in the models.

Models Used in Initial Environmental Exposure Assessment

24. Three local models on a national scale for estimation of the concentration of a chemical in air phase, six for water phase (including a simple dilution model which does not require PCs for calculation), and two for soil phase were submitted for distribution by Member countries. Eight of them, which are thought to be simple but appropriate for use for an initial assessment of HPV chemicals with full SIDS, are included in diskettes. Also four fugacity type global national models are available through diskettes.

25. As various modelling approaches are taken by Member countries, a set of four so-called "reference models", namely the Screening Assessment Model System (SAMS) which consists of three local models (Water, Air and Soil) and one global model (Fugacity Model, FUGMOD), have been developed. The basis and mechanisms considered have been agreed at the Workshop. They serve as a minimum assessment procedure, but Member countries could use them in addition to or in place of their own approaches. The choice of which of the three local models to use will be made on the basis of the compartments identified as receiving the release of the chemical. Detailed information on reference models is presented in Annex 2 to this document, and reference models developed are available through a diskette.

26. By using local models, Member countries should be able to have opportunities to adapt the input data to their own particular situation. The possibility of developing a reference scenario which represents generic local conditions should also be investigated. A conservative approach to the choice of generic parameters should be taken.

27. Even for a chemical used in closed systems,[**] estimation of the amount of the chemical that can be expected to reach the environment can be carried out. An approach presented in the MNSEM model based on the physical-chemical properties can be considered as one of the methods that can be applied.

28. FUGMOD, which is the latest version of the Fugacity Level III model, is to be used as the basis of the global models. The default environmental parameters for this version also could be used in the assessment in addition to, or in place of, parameters for the environment of each country. This global reference model is available on a diskette.

29. Currently there are various models which can be identified for use in environmental exposure assessment. However, to date there is a lack of standardisation of selection of distribution models employed for the initial assessments. Harmonization in this field would be desirable.

30. Methods used, including any assumptions made, extra data required, and QSAR estimation adopted, should be transparent to others in order to undertake the assessment of HPV chemicals in a co-operative way.

31. It is the responsibility of the user of the models to assess the effect of uncertainties in the data when estimation is carried out by the models.

4.3.4 Models for Indirect Exposure by Food and Drinking Water

32. Exposure of human beings is generally expressed as an average daily intake of a chemical per unit of body weight. In the initial indirect exposure assessment this average daily intake of a chemical is compared with the "low risk level of average intake", which is derived from the results of toxicity testing and other information. Models for indirect exposure by food and drinking water are used for estimation of the average daily intake using default values, the data for intake volume of food, drinking water and air, and concentrations of chemicals in the media. Therefore there is a close relation with environmental exposure models and indirect exposure models. Some models consist of both a model for

[**] A chemical used in closed system: a substance should only be considered to be used in closed systems if it remains within a reactor or is transferred from vessel to vessel through closed pipework and therefore accidental spillage is the only likely cause for human exposure or environmental contamination.

environmental exposure and a model for indirect exposure in order to conduct an assessment in an integrated way. An elaborated exposure assessment would be required in cases where estimated intake exceeds the "safe level of average intake."

33. "Indirect Exposure of Human Beings to Organic Chemicals" (Ref. 18 and 38) summarises the approaches of Member countries. Four national models which are compiled on the diskette could be used for estimation. Also estimation of indirect exposure could be done partly by reference models.

Necessary Information

34. Physical-chemical data in the SIDS are thought to be sufficient for the models submitted by Member countries, but further data on the estimation of emission beyond data included in the SIDS are considered to be necessary.

Models

35. Four models (CHEMCAN, CHEMFRANCE, MNSEM, and RISK) are adaptable to individual country needs and are available for those Member countries who wish to use them in their initial indirect exposure assessment of HPV chemicals to humans. All of them are available through diskettes. In addition, reference models could be used for partial estimation of indirect exposure.

36. Both local and global approaches should be used when circumstances indicate that this type of insight would be useful to the assessment.

37. The indirect exposure assessment should cover critical target groups such as children and elderly people.

38. Calculations for extreme dietary compositions such as high and low consumption of fish should be carried out if available information suggests this is important.

Annex 1

Emission Factors and Use Categories of Chemicals

(Summary Report of Working Group I of the OECD Workshop held in Berlin in December 1991)

Objectives and Purpose of the Working Group

1. Environmental release estimation is the first step within the exposure assessment. Release estimates involve the identification of the sources and the receiving environmental media for each stage of the chemical's life cycle. Specific quantities released during these stages can be expressed as emission rates or emission factors. The objective of release assessments is to develop information that provides a starting point for estimating chemical concentrations in media of concern. Working Group I considered issues related to releases before and after waste water treatment. It was agreed that water releases of SIDS chemicals will be estimated before and after waste water treatment.

Information and Data Sources for Developing Release Assessments

2. The Discussion documents (Ref. 14 and 15) and the Background documents (Ref. 20, 24 and 29) developed for the Workshop were presented. The documents detail:

- databases containing chemical release information;
- sources for obtaining emission factors for chemicals;
- approaches for estimating releases used in the EC and US new chemicals programmes.

3. In addition, nine Member countries provided estimates of releases and exposures for nine selected SIDS chemicals. These submissions also provide insight into methods that numerous Member countries use to estimate chemical releases.

4. Most participants agreed that initial exposure assessments should be based on the SIDS dossier with the understanding that it may be necessary to get additional exposure information on chemicals of concern after the initial assessment. Participants from one Member country were concerned that initial assessment of SIDS chemicals may be impossible given the information in the SIDS dossier. Participants from a number of Member countries indicated they would assure that their assessments would be based on information beyond what is available in the SIDS Dossier. Participants from other Member countries expressed their anxiety that they may not have the resources to obtain additional information, though they have extensive dialogue with industry for each SIDS chemical. Therefore, they may prefer a screening assessment which uses only SIDS Dossier data or accepted worst case assumptions in order to complete the SIDS screening on a timely basis.

5. The Working Group recommended that Member countries take advantage of mandatory release reporting requirements or other data sources of several Member countries. Product registries are an example of this kind of relevant data. It was recommended that Member countries strive to use as much as possible monitoring data, such as that available in the literature and databases, whenever appropriate in their release and exposure assessments. Assessments based on monitoring data should be compared to estimates using other approaches. The Working Group recommended that release assessors should involve waste management officials in the development of their assessments. In addition, chemical manufacturers may be able to provide more detailed information on chemical use and releases. The Working Group was aware that the further downstream a release scenario was from manufacturing, the poorer the use information may be supplied by the manufacturer.

Life-cycle Assessment and Relevant Emission Scenarios

6. There was agreement that releases should be assessed for the entire life-cycle of SIDS chemicals. The life-cycle of a chemical includes:

-- manufacture or production;
-- processing or formulation;

-- industrial use;
-- private or consumer use;
-- recycling;
-- disposal and waste treatment.

7. For commonly encountered release scenarios, estimates of releases may be based on working models and might take the form of the matrix shown in the Appendix to this Annex which shows releases as a fraction of production or use volume.

8. It was agreed that an iterative approach to improving initial assessments may be needed on occasion.

9. There was concern in the Working Group that many release estimating models are based on estimates of production or use volumes which are not necessarily of high quality.

Scope of SIDS Release Assessments

10. There was general agreement that all SIDS release assessments should be extremely clear with regard to how they were developed and should, when possible, include:

-- rationales, assumptions and data used to generate release estimates;
-- types of releases (point source or diffuse);
-- release quantities;
-- media for release;
-- time dimensions of releases;
-- kinds of release estimates (average or worst case);
-- uncertainties associated with the estimates.

Results of Comparison of Release Estimating Methods for Selected SIDS Chemicals

11. The Working Group considered release and exposure estimates for the selected chemicals as submitted by nine Member countries. Member country approaches to estimating water releases of chemicals were often conceptually similar. However, differences in values chosen for variables contained in release calculations frequently lead to widely varying release concentrations. This situation probably exists for other release scenarios that may be evaluated in the future. There is a clear need for the Member countries to work more closely together to develop mutually compatible release estimating methods.

12. It was generally agreed that the SIDS assessment efforts should be structured to avoid false negatives - incorrectly excluding chemicals of potential concern from further consideration. False positives should be identified during the exposure assessment process.

Applicability of New Chemical Assessment Methods to the SIDS Programme

13. Patterns of the intended use are usually well known for new chemicals. For HPV chemicals, use patterns may not be easily identifiable. For some Member countries this means that assumptions, such as default values, may be more commonly relied on for HPV chemical assessment than for new chemical assessment.

Summary of Conclusions and Recommendations

14. Even though it was not possible for the Working Group to develop consensus decisions regarding the details on how to estimate releases for selected scenarios, there were many useful results. The most significant were:

14.a Many relevant release assessment tools were distributed to the participants through the Discussion documents and the Background Document. These tools will assist Member countries in developing release assessments as well as allow them to understand the assessments of other Member countries. Additional assessment methods, use category documents, and other materials not yet submitted from other Member

countries should be exchanged through the OECD. The OECD should endeavour to expand the Working Group Background Document to include additional assessment tools available in other Member countries and make it available.

14.b There was agreement that releases should be assessed for the entire life-cycle of SIDS chemicals. The life-cycle of a chemical includes:

- -- manufacture or production;
- -- processing or formulation;
- -- industrial use;
- -- private or consumer use;
- -- recycling;
- -- disposal and treatment.

14.c There was agreement that all SIDS release assessments should be extremely clear with regard to how they were developed and should, when possible, include:

- -- rationales, assumptions and data used to generate release estimates;
- -- types of releases (point source or diffuse);
- -- release quantities;
- -- media for release;
- -- time dimensions of releases;
- -- kinds of release estimates (average or worst case);
- -- uncertainties associated with the estimates.

14.d Member country approaches to estimating SIDS chemical intermediate water releases, were often conceptually similar. However, differences in values chosen for variables contained in release calculations frequently lead to widely varying release concentrations. This situation probably exists for other release scenarios that may be evaluated in the future. There is a clear need for the Member countries to work more closely together to develop mutually compatible release estimating methods.

14.e Release assessments will address releases up through waste water treatment. Water releases of SIDS chemicals will be estimated before and after waste water treatment.

14.f For many use categories there are no adequate emission scenarios. Member countries should develop and share use category information and other assessment tools.

APPENDIX TO ANNEX 1

Industrial Category	**Use category / Function**	**Release Estimates**				**Applicable Steps of Life Cycle**
		Water	**Air**	**Soil**	**Waste**	
1. Agricultural chemicals	Fertilisers Pesticides					Production Compounding Processing Use (private) Recovery
	Pharmaceutical (vet.)					Production Compounding Processing Use (private) Recovery
2....						

. . 15....						

- Diffuse
- Local: point source (fraction, time periods,...)

Annex 2

Local and Global Models

(Summary Report of Working Group II of the OECD Workshop held in Berlin in December 1991)

Objectives

1. The objectives of the Working Group were to identify and recommend suitable environmental models for use in initial screening assessment. Appropriate models would provide estimates of concentrations in environmental compartments of concern (Predicted Environmental Concentration, PEC). Additional information on mass balances, mass fluxes or residence times from the models would be valuable for a better understanding and evaluation of the fate and pathways of the chemicals. The models should be able to use release estimates from Working Group I and the data available in the SIDS.

Scope of the Models

2. A range of modelling approaches was used by Member countries in the estimates carried out in preparation for the workshop. These are summarized in Background Documents (Ref. 21 and 22). It was obvious from the discussions in the Working Group that different Member countries had different methods which they would like to use. The approach agreed therefore was to find a set of models which would act as a minimum assessment procedure, but which Member countries could use in addition to, or in place of, their own approaches.

3. It was agreed that the Working Group should aim to recommend models which covered the range of spatial and temporal scales over which assessments are carried out. After discussion a set of four models was decided upon - three local models, each concerned with a single environmental phase (Air, Water, Soil), and one global model. For the purposes of this document, local models are those which are concerned with the environment close to the release site, and with a short time scale after the release. They can use environmental data which is generic or they can use data from a real situation if such information is available. The choice of which of the three local models to use would be made on the basis of the compartments identified as receiving the release of the chemical. Global models are those which are concerned with the longer term, steady state behaviour of a chemical, and are multi media. The scale of those models favoured by the group was national or regional.

Description of Models

4. It was agreed at the beginning of the discussions that the aim would be to identify the key processes involved and the data requirements (both for the chemical and the environment). As far as possible the chemical data should be available from the SIDS or through the SAR methods discussed in the Special Session on SAR. It was decided that only the basis of the models would be recommended and not actual models for use. The discussion was based on the Discussion Document (Ref. 16 and 19).

Local Models

a. Water model

i. Major processes: dilution.

ii. Optional processes: volatilization, degradation, adsorption.

iii. Chemical data: release rate (mass/time, mass/site/time), release concentrations and discharge flows, Henry's Law Constant, Bioconcentration Factor (BCF), Organic Carbon Sorption Constant (Koc).

iv. Environmental data: flow rates (generic or site specific).

v. Remarks: Calculation of dilution is the minimum necessary. Member countries may then use the concentration obtained in order to calculate concentrations in sediment, biota etc. through the appropriate physical-chemical data. They may also use the available data to indicate whether reductions in this concentration through degradation, volatilization are likely.

[Note:

i. Major processes: the processes which should be considered in the Models.
ii. Optional processes: the processes which can be considered optionally in the Models.
iii. Chemical data: the physical-chemical data of a chemical which are necessary for calculation by the Models as input data.
iv. Environmental data: the data on the environment for which the calculation is carried out.]

b. Air model

i. Major processes: dispersion, dilution.

ii. Optional processes: degradation, deposition.

iii. Chemical data: release rate (mass/time). No other data required for basic assessment; degradation and physical-chemical data may be used to modify the assessment.

iv. Environmental data: source height, mixing layer height, meteorological parameters; for all these, generic or site specific information could be used.

v. Remarks: The calculation of dilution is the minimum necessary. The approach for calculation of concentrations is dependent on the type of release. For a point source, a local plume model should be used. A modification of this could be used to describe a larger area source, for example a city. For other types of source a box model may be more appropriate. Member countries should use their judgement in choosing which method to apply. The results required are the concentration in the plume where it first interacts with the ground or with a receptor of interest, or the distributed concentration in the box model. Degradation and physical-chemical data may be used to indicate whether changes in the calculated levels are likely. They could also be used to estimate deposition rates for use as input into the soil model.

c. Soil model

i. Major processes: partitioning between water and soil; removal by degradation, leaching.

ii. Optional processes: volatilization, root uptake.

iii. Chemical information: Henry's Law Constant, Koc, degradation rate(s), deposition rate, concentration in sewage sludge.

iv. Environmental data: soil properties (porosity, water content, organic carbon content, depth of root zone and surface layer (see remarks)); meteorological properties (rainfall, evaporation, or a water balance).

v. Remarks: This situation is more complicated than the previous two models. Two possible release routes were considered: deposition from air, or application of sewage sludge containing the chemical. Member countries may consider other release routes if they so wish. It was agreed that concentrations were desired to assess effects on soil organisms and on possible levels in groundwater. Accordingly there are actually two versions of the same model that may be used here. For assessing effects on soil organisms, a model of only the shallow surface layer might be considered. For levels in groundwater, calculations would be carried out for soil to the depth of the root zone or below; the concentration in the leaching water would be then available for use in assessing groundwater concentrations. Different values for organic carbon content etc. could be used for the two cases. Values for the depths of the two layers, and the soil properties should be chosen by the Member countries (generic or site specific). The possibility of volatilization affecting the estimated concentrations was considered, but it was felt that the routes of release had already taken this into account.

General Comments on the Local Models

5. Throughout these models there are opportunities for Member countries to adapt them to their own particular situations. Whilst it was agreed that this should be done where the data was available, it was felt by several of the participants that the application of a set of generic local conditions as a reference scenario would also be useful. It is recommended that the possibility of developing such scenarios be investigated. It is also recommended that Member countries take a conservative approach to the choice of generic parameters.

Global Model

6. Rather than derive a multi media model from basic processes, the group decided after discussion that the Mackay level III model should be used as the basis of the global model. However, this did not rule out the use of other models considering long term fate if a Member country had such models available.

7. As a number of versions of this model have been available over the years, it was agreed that it was important that all Member countries had the same basic model with which to work, if they wished to use this approach. The version chosen was that presented by Frank Wania (University of Toronto) at the Workshop, and described in "Generic Models for Evaluating the Regional Fate of Chemicals" by D. Mackay et al. (*Chemosphere*, in press 1992) (Ref. 34). This should be adapted to model the environment of the Member country if this was possible, for example by using appropriate sizes for the compartments. If this was not possible, the default compartment sizes as presented in the article should be used. In line with the comment above on the local models, it was felt by many of the participants that it would be useful for each country to use these default values in addition to their own values if possible. In order to allow Member countries to modify the environmental parameters, development of a modified version of the computer program was necessary.

i. Chemical data required: physical-chemical data from the SIDS data set; degradation rate data, release rate appropriate to the model used.

ii. Environmental parameters: compartment volumes, areas, densities, organic carbon content where appropriate. These are the parameters which users can input in the modified version.

iii. Remarks: Where parameters such as Koc, BCF are estimated from other data it is important that the method used is indicated. This is also the case for estimates of degradation rate. For the generic model, an appropriate input rate should be used, for example 1% of the total release in the OECD Member countries.

General Remarks

8. It is important when using the approaches indicated above that any assumptions made or extra data used are made clear, for example the reasons for choosing flow rates in the water model should be given. If SAR methods are used to estimate other data, the method used should be given. It is essential that the methods used are transparent to other Member countries.

9. The physical-chemical data available in the SIDS are generally sufficient for these models. For some data it is necessary to use SAR methods.

10. There is a general lack of information on degradation rates in the SIDS data set. This may not be important for the local models in the first instance, but it is an obvious problem for global models. Therefore the Working Group recommends that efforts be made to improve the provision of such data, whether through measurement or estimation.

11. Where there are uncertainties in the data used, the user should assess the effect these have on the concentration estimates. In addition it should be noted that there are some chemicals for which these methods are not suitable.

12. It is recommended that models based on the methods in this report should be developed and distributed to Member countries by the OECD Secretariat in time to perform the next round of assessment of HPV phase 1 chemicals. Member countries are invited to submit their own models to be distributed at the same time.

Annex 3

Models for Indirect Exposure by Food and Drinking Water

(Summary Report of Working Group III of the OECD Workshop held in Berlin in December 1991)

1. The objectives of the Working Group were to identify and recommend suitable models for indirect human exposure assessment. It was generally agreed that such models cannot be considered separate from models used for estimating environmental concentrations. Therefore, discussions touched parts of the discussion in Working Groups I and II, especially concerning the scale on which indirect exposure of human beings is considered.

2. The main discussion point concerned the connection between environmental models and indirect exposure models. The exact process descriptions were seen as of minor importance, as they are more or less the same in most models.

Models presented

3. There were six models presented by the members of the Working Group.

3.a CHEMCAN 2 (Canada, Ref. 1)

i. This is a global model based on Mackay Level III dividing Canada into 24 regions considering four primary (air, water, soil, sediment) and four secondary compartments (groundwater, coastal water, terrestrial plants and terrestrial animals).

ii. Indirect exposure of humans can be calculated from the concentrations in food but up to now it is not included in the model. Fine tuning of some pathways (e.g. soil-plant) has to be carried out.

3.b CHEMFRANCE (France, Ref. 3)

This model is similar to CHEMCAN 2 dividing France in 12 regions.

3.c MNSEM (Japan, Ref. 5 and 6)

This model is also similar to CHEMCAN 2, that means it is also based on Mackay Level III and it is specific for Japan. It calculates concentrations for all relevant compartments as well as the total daily intake for adults. Elimination according to first order kinetics can also be calculated.

3.d RISK (Netherlands, Ref. 7)

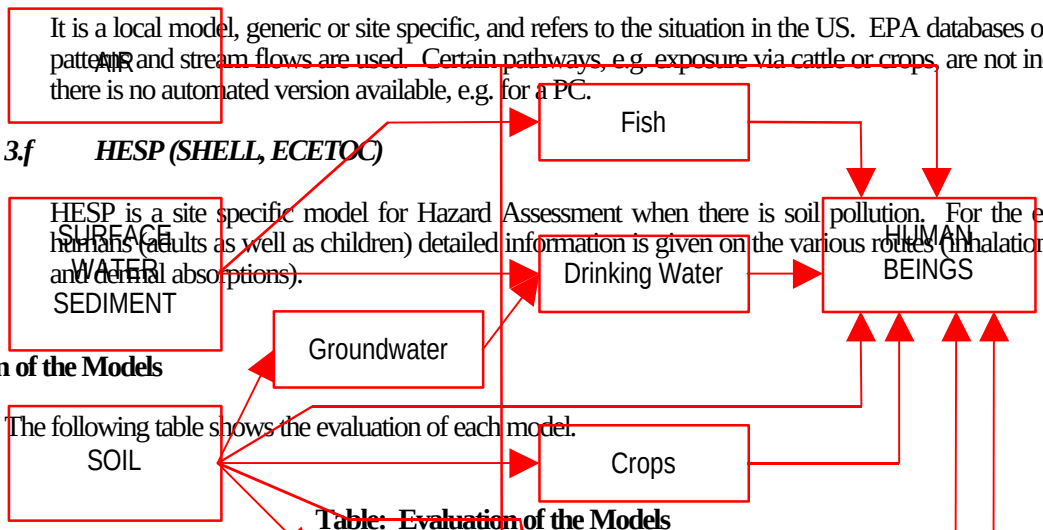
RISK is a local model for a generic standard environment and is specific for average conditions in the Netherlands. It is a worst case approach for indirect exposure of humans, but can be modified to a realistic worst case.

3.e US Approach (Ref. 11 and 22)

It is a local model, generic or site specific, and refers to the situation in the US. EPA databases on emission patterns and stream flows are used. Certain pathways, e.g. exposure via cattle or crops, are not included and there is no automated version available, e.g. for a PC.

3.f HESP (SHELL, ECETOC)

HESP is a site specific model for Hazard Assessment when there is soil pollution. For the exposure of humans (adults as well as children) detailed information is given on the various routes (inhalation, ingestion and dermal absorptions).



Evaluation of the Models

4. The following table shows the evaluation of each model.

Table: Evaluation of the Models

NAME	Scale	Input data	Data covered by SIDS
CHEM-FRANCE	global, specific for France	physical-chemical emission estimates	+ -
CHEMCAN 2	global, specific for Canada	physical-chemical emission estimates	+ -
MNSEM	global, specific for Japan	physical-chemical emission estimates	+ -
RISK	local, generic	physical-chemical emission estimates	+ -
US Approach	local, generic or specific	physical-chemical emission estimates	+ -
HESP	site specific	physical-chemical soil concentration	+ -

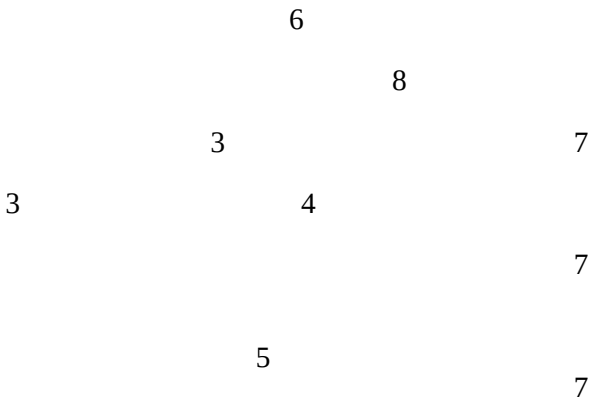
5. For all models emission estimates or soil concentrations are necessary but not available from SIDS.

6. The structure of indirect exposure models as proposed in Figure 1 of the Discussion document (Ref. 18) was agreed. One amendment is proposed by adding SEDIMENT as a pathway to FISH.

1

2 7

6 7



1 inhalation	3 bioconcentration soil-plant	5 biotransfer to milk	7 consumption
2 bioconcentration water-fish	4 biotransfer to meat	6 purification of drinking water	8 ingestion of soil

Figure 1 - Schematic Representation of the Indirect Exposure to Human Beings

Conclusions

7. It was stressed that because certain target groups like children or elderly people behave differently from the average adult, it is important that such critical target groups be included in indirect exposure assessments. There may be also large differences between the exposure of communities which live near the source compared to the population as a whole.

8. All models except HESP are in fact environmental models which include modules/methods for estimating human intake. This emphasizes the strong relationship with the local and global models as discussed in Working Group II. HESP is the only true human exposure model, developed for specific application. Four models namely CHEMCAN, CHEMFRANCE, MNSEM and RISK have been developed for specific regions. They are adaptable and, therefore, are available to those Member countries who wish to use them in their initial indirect exposure assessment of HPV chemicals to humans.

9. Both local and global approaches were thought to be important in order to obtain insight into the exposure of local and average populations. Both types of models are strongly recommended to be used, when circumstances indicate that this type of insight will be useful to the assessment. Similarly, to the extent warranted by other factors or information, it is recommended to carry out calculations for extreme dietary compositions, e.g. high and low consumption of fish, meat or vegetable.

10. It was considered that the US approach is not so easily adaptable and, therefore, is of limited use to other Member countries. HESP can be used only for specific purposes (soil contamination) and is therefore out of scope for the initial exposure assessment of HPV chemicals of the OECD Existing Chemicals Programme.

Annex 4

References

A. Member Countries' Responses to the Questionnaire

1. Application of a Fugacity-Based Model to the Estimation of the Environmental Fate of 10 Chemicals on the OECD SIDS List, J. Sitwell and D.M. Kane, National Health and Welfare (Canada)

2. Environmental Exposure Assessment, Product Register Data on Ten Selected Substances, P. Andersen, National Institute of Occupational Health (Denmark)

3. Environmental Behavior of Ten Organic Compounds, J. Devillers and D. Domine CTIS (France)

4. Response from Germany, P. Greiner, Umweltbundesamt (Germany)

5. Application of Simple Model for Environmental Exposure Assessment, K. Yoshida, Mitsubishi-kasei Institute of Toxicological and Environmental Sciences (Japan)

6. Multi-Phase Non-Steady State Equilibrium Model (MNSEM) Version 1.4.5 Model Information, K. Yoshida, Mitsubishi-kasei Institute of Toxicological and Environmental Sciences (Japan)

7. Assessment of Environmental Concentrations and Risk Quotients for the Netherlands: Application of Simple Models, C. Toet, D. van de Meent, Th.E.M. ten Hulscher, K.D. van den Hout, National Institute of Public Health and Environmental Protection etc. (the Netherlands)

8. Environmental Exposure Assessment, E. Hoygaard, State Pollution Control Authority (Norway)

9. Initial Exposure Assessment of 10 HPV/P1 Chemicals, Applying a Swedish Exposure Model (Revised version), S. Fischer, National Chemicals Inspectorate (Sweden)

10. Response from United Kingdom, P.J. Corcoran, Department of the Environment (United Kingdom)

11. Engineering and Environmental Exposure Report for Ten High Production Volume SIDS Chemicals, (US Environmental Protection Agency)

B. Request and Data on the Ten SIDS Chemicals

12. Data on ten selected SIDS Chemicals from HPV Form 1 (OECD Secretariat)

13. Estimates of Ecotoxicity (Aquatic Effects) and Bioaccumulation, Data of the Ten SIDS Chemicals (the Netherlands)

C. Discussion Documents for the OECD Workshop held in Berlin in December 1991

14. Emission Factors and Use Categories of Chemicals (for W.G.I) (W. Penberthy, P. Greiner)

15. Memorandum: OECD Scheme for Estimating Rates of Removal in Waste Water Treatment (for W.G.I - comments on Ref. 14 by the US) (R. Boethling)

16. Local and Global Models (for W.G.II) (OECD Secretariat)

17. Application of SARs to the Estimation of Properties Important in Exposure Assessment, Fraunhofer - Institute (for the Special Session) (P. Degner, H. Jackel, M. Muller, N. Nendza, B. von Oepen, W. Klein)

18. Indirect Exposure of Human Beings to Organic Compounds (C. Toet, S. Arai)

19. Reference Models which would be used for the Initial Environmental Exposure Assessment (for W.G. II) (M. Matthies)

D. Background Documents for the OECD Workshop held in Berlin in December 1991

20. Emission factors and Use Categories of Chemicals (for W.G.I) (W. Penberthy, P. Greiner)

21. Local and Global Models (for W.G.II) (OECD Secretariat)

22. Potential Approaches for Developing Screening-Level Environmental and Human Exposure Assessments for SIDS Chemicals (for W.G.II) (E. Bryan)

E. Additional References

23. OECD's Work on Investigation of High Production Volume Chemicals, OECD, 1991

24. Environmental Releases of Chemicals in Household Products, US EPA, Dec. 1991

25. Site-Specific Surface Water Flows and REACH Number, US EPA, Dec. 1991

26. Stream Dilution Factor Programme Outputs for 40 Industrial Categories, US EPA, Dec. 1991

27. User's Guide to Probabalistic Dilution Model 3 (PDM 3), US EPA, Dec. 1991

28. Probabalistic Dilution Model 3 (PDM3), US EPA, Dec. 1991

29. A Model of Organic Chemical Fate in a Biological Wastewater Treatment Plant, B. Clark et al. University of Toronto, Oct. 1989

30. Comparison of different models for Environmental Hazard Classification of Chemicals, KEMI Report No. 9/89

31. Systems for Testing and Hazard Evaluation of Chemicals in the Aquatic Environment, A Manual for an Initial Assessment - ESTER, KEMI Report No. 4/88

32. Substances and Preparations Dangerous for the Environment, A System for Classification, Labelling and Safety Data Sheets, Final Report from a Nordic Working Group, Nordic Council of Ministers, 1990

33. Fugacity Models, D. Mackay et al., Practical Application of QSAR in Environmental Chemistry and Technology , June 1990, Klamer Academic Publication, pp. 433-461

34. Generic Models for Evaluating the Regional Fate of Chemicals, D. Mackay et al. (Chemosphere, in press 1992)

35. The Explanatory Note for Diskettes Comprising National Models, OECD Secretariat, July 1992

36. Screening Assessment Model Systems ("SAMS", The Explanatory Note for Diskette of the Local Reference Models, Version 1.1), OECD Secretariat, December 1992

37. The Explanatory Note for Diskette of the Global Reference Model, OECD Secretariat, July 1992

38. Report of the OECD Workshop on the Application of Simple Models for Environmental Exposure Assessment, Environment Monographs No. 69, 1993

39. Application of Structure-Activity Relationships to the Estimation of Properties important in Exposure Assessment, Environment Monographs No. 67, 1993

F. List of Diskettes and Documents Distributed to the SIDS Contact Points

a. Reference Models and National Models (ENV/EHS/SA/fcl/92.40, 11th August 1992, and ENV/EHS/SA/fcl/93.1, 11th January 1993)

- Diskettes of Reference Models ("Screening Assessment Model System (SAMS)" Version 1.1 and "Fugacity Model (FUGMOD)")
- Two diskettes of National Environmental Exposure Models (i.e. The Netherlands, UK, Canada, France and Japan)
- Explanatory Note of a Diskette of the Global Reference Model (FUGMOD)
- Explanatory Note of a Diskette of the Local Reference Models (SAMS Version 1.1)
- Explanatory Note of Diskettes Comprising National Models

b. Documents and Diskettes of the U.S. models (ENV/EHS/SA/fcl/92.41, 11th August 1992)

- A letter from Ms. E. Bryan to Rob Visser dated 23rd March 1992

- Models

1. STP (Sewage Treatment Plant model or "Toronto model")
   - The diskette of "Water" includes STP

2. Water (the following sub models)

   A. Exposure from Airborne Release
      a. Turner model
         - Enclosure I of the letter: Document for Generic Turner Method for Estimated Exposure from Near-Ground Releases to Air
      b. ISCLT model (Industrial Source Complex Long Term model)
         - Enclosure II of the letter: Documentation for Generic ISCLT Method for Estimating Exposure form Elevated Release to Air
   B. Site-specific Surface Water Release Calculation
   C. Industrial SIC- Code Based Water Surface Water Calculation
   D. Drinking Water Exposure from Landfilled Chemicals
      - Enclosure III of the letter: Draft Guidelines for Groundwater Assessments for PMN Chemicals
   E. Chemical Removal from Adsorption

   Diskette
   - Water (including above mentioned six models)
   - STP (Toronto Model)
   - PMNPLUME Model

3. PMNPLUME
   - PMNPLUME Exposure Model Description and Use's Manual
   - The diskette of "Water" includes PMNPLUME

4. Probabilistic Dilution Model 3 (PDM3)
   - Draft Report, Probabilistic Dilution Model 3 (PDM3), Volume 1 and 2
   - Final report, User's Guide to PDM3
   - Diskettes "PDM3" (6 diskettes for a set)
     1. Option 1 Estimated flows
     2. Option 1 Measured flows, disk 1 of 3
     3. do , disk 2 of 3
     4. do , disk 3 of 3
     5. PDM.EXE
     6. Option 2 SIC code data

5. ReachScan

- ReachScan User's Manual
- a diskette of ReachScan with Region 3 Stream Data

6. PCGEMS
   - PCGEMS User's Guide Release 1.0
   - Diskettes for PCGEMS (21 diskettes for a set)